C23

Beyond Potential Energy Surfaces: A Quantum Geometric View of Molecular Electronic Structure

A. Pausch[1]

[1] *Universität Münster, Germany*

Quantum geometry has become a central language in modern condensed matter physics. Its central quantity, the quantum geometric tensor, characterizes how the wavefunction varies with changes in external parameters, thereby providing a unified description of the coupling between a quantum system and its environment. This perspective has proven instrumental in understanding phenomena ranging from anomalous Hall conductance to the Aharonov–Bohm effect. Molecular quantum chemistry, by contrast, is still formulated primarily in terms of energies, gradients, and potential energy surfaces. Yet the same quantum geometric structures arise naturally when electronic states are viewed as functions of nuclear coordinates, electromagnetic fields, or other external parameters. In this contribution, I will highlight that quantum geometry provides a complementary language for molecular electronic-structure theory, revealing that a variety of seemingly distinct molecular response properties are, in fact, manifestations of the same underlying quantum geometric tensor. Whenever observables depend on derivatives of the electronic wavefunction, geometric contributions naturally emerge. Examples include corrections beyond the Born–Oppenheimer approximation, magnetic response phenomena, and several forms of vibrational spectroscopy.

Recent methodological advances have made these quantities accessible within established quantum chemical frameworks. Linear response current-density functional theory now enables the evaluation of the full molecular quantum geometric tensor for a broad range of density functional approximations, extending its application to regimes such as strong magnetic fields. Here, the Berry curvature enters the nuclear equations of motion as a Lorentz-like force, enabling quantitative descriptions of molecular dynamics and rovibrational spectroscopy. These results demonstrate that molecular motion is governed not only by the potential energy surface, but also by the geometry of the underlying electronic wavefunction itself. Taken together, these developments establish quantum geometry as an organizing language for electronic response, nuclear motion, spectroscopy, and external perturbations. The same perspective naturally extends beyond isolated electronic states: degenerate state manifolds require non-Abelian geometric structures, opening routes towards unified, gauge-covariant descriptions of coupled electronic, spin, and nuclear dynamics. Molecular quantum chemistry may therefore benefit substantially from adopting a geometric viewpoint that has already transformed condensed matter theory.